

2006 Listing of Material Science PI Publications

Palosz, W., "Vapor transport of ZnO in closed ampoules," *Journal of Crystal Growth*, 286, 42-49, 2006.

Dr. Palosz is with BAE Systems/MSFC and is the Principal Investigator for the ground-based project "Investigation of "Contactless" Crystal Growth by Physical Vapor Transport."

Vapor transport of ZnO by PVT and CVT using carbon, carbon monoxide and hydrogen as the transport agents was studied. Theoretical calculations of the mass flux were based on equilibrium thermodynamics and 1D diffusional mass transport. Experimental results were found to be consistent with theoretical predictions. No apparent kinetic limitations to sublimation or CVT processes were observed. Slow reaction of carbon with ZnO source was found.

Binici, Burcu, Dionne I. Fortenberry, Kayce C. Leard, Marcus Molden, Nesrin Olten, Sam Popwell and **John A. Pojman**, "Spherically Propagating Thermal Polymerization Fronts," *Journal of Polymer Science: Part A: Polymer Chemistry*, 44, 1387-1395, 2006.

Dr. Olten is at Kocaeli University, Turkey, and Ms. Fortenberry at Mississippi University for Women. The other authors are at University of Southern Mississippi where Professor Pojman is the Principal Investigator on the project "Transient Interfacial Phenomena in Miscible Polymer Systems," which has just been transitioned from flight to ground status, having passed its Science Concept Review.

We demonstrate for the first time spherically propagating frontal polymerization that also exhibits spin modes. We have developed an interesting system using the amine-catalyzed Michael addition of a trithiol to a triacrylate to create a rubbery gel. The gel suppresses convection and bubble formation during front propagation. A peroxide is also present to act as a thermal initiator. The front propagates via free-radical polymerization of the remaining triacrylate after being initiated photochemically in the center of the reactor. It is possible to prepare the rubbery gel in any shape and the initiate thermal frontal polymerization. So-called spin modes have been observed for the first time in spherically propagating fronts in which waves of polymerization propagate on the expanding spherical front. A system using a diacrylate dissolved in dimethyl sulfoxide with added gel and with persulfate as the initiator supports spherical fronts but does not exhibit spin modes.

McFarland, Brian, Sam Popwell, and **John A. Pojman**, "Free-Radical Frontal Polymerization with a Microencapsulated Initiator: Characterization of Microcapsules and Their Effect on Pot Life, Front Velocity, and Mechanical Properties," *Macromolecules*, 39, 55-63, 2006.

The authors are at University of Southern Mississippi where Professor Pojman is the Principal Investigator on the project “Transient Interfacial Phenomena in Miscible Polymer Systems,” which has just been transitioned from flight to ground status, having passed its Science Concept Review.

In this study, microcapsules containing a cumene hydroperoxide (CHP) core were produced by interfacial polymerization and tested in a variety of free-radical frontal polymerization systems. It was observed that the microcapsules could be used successfully in number of systems, and comparisons were made with typical frontal polymerization systems. The effect of encapsulation of CHP on the pot life was tested in a variety of systems, and it was observed that systems containing microcapsules underwent a dramatic increase in pot life, from hours to weeks in certain systems and from a few days to several weeks in other systems. Polymer samples that were produced from 1,6-hexanediol diacrylate (HDDA) systems with and without microcapsules were tested for modulus and toughness. It was observed that the use of CHP microcapsules resulted in an increase in the modulus and toughness (up to 2x) of polymer samples.

Mendoza, R., K. Thornton, I. Savin, and **P. W. Voorhees**, “The evolution of interfacial topology during coarsening,” *Acta Materialia*, 54, 743-750, 2006.

The authors are at Northwestern University, where Professor Voorhees is the Principal Investigator on the ground -based project “The Evolution of Dendrite Morphology during Isothermal Coarsening.”

Quantitative characterization of coarsening is achieved through topological measurements such as the genus, the number of handles, and the number of independent bodies (liquid droplets). Topological analysis was performed on experimentally derived, three-dimensional reconstructions of dendritic microstructures. Measured topological quantities were reported on a per volume basis and scaled by the length scale of the system to remove effects of the changing length scale during coarsening. The scaled genus decreased with coarsening time due to the simplification of the topology of the microstructure, while the number of liquid droplets increased with coarsening time. These results were supplemented with calculations of the interfacial velocity determined using phase-field simulations that employ the experimental three-dimensional reconstructions as the initial condition. Through these calculations it is shown that liquid droplets form through capillary-driven instabilities of interconnected liquid channels, while liquid tubes are created through topological singularities occurring on large planar-like walls of liquid.

Khine, Y. Y., and **R. M. Banish**, “3D mass diffusivity model of liquid metals in the presence of a magnetic field,” *Journal of Crystal Growth*, 287, 287-290, 2006.

The authors are at University of Alabama in Huntsville, where Dr. Banish is the Principal Investigator on the ground-based project “Temperature and Composition Dependence of Mass and Thermal Diffusion in Liquid Metals and Compound Semiconductor Alloys.”

The effect of convective contamination for mass diffusivity measurements of liquid germanium with moderate and strong magnetic fields is analyzed in three-dimensional (3D). A steady-state, 3D temperature profile that represents a heat flux at the sidewall varying as $\cos(\theta)$ in the azimuthal direction is imposed on the cylinder. The temperature non-uniformity-driven convective contamination that leads to approximately 5% greater mass flux, or an allowable temperature non-uniformity is determined for magnetic field strengths of 0.75 and 4.5 T. From the numerical results, the temperature non-uniformity that liquid germanium can tolerate is a tenth of a degree or less for all the cases. The velocities are directly proportional to the temperature non-uniformity in the liquid, with axial velocities usually an order of magnitude higher than the radial and azimuthal velocities. A stronger magnetic field can allow a larger temperature non-uniformity for the same heat transfer condition.

Woods, Vincent, and **Nikolaus Dietz**, "InN growth by high-pressures chemical vapor deposition: Real-time optical growth characterization," *Materials Science and Engineering*, B127, 239-250, 2006.

The authors are at Georgia State University where Dr. Dietz is the Principal Investigator on the ground-based project "Optical characterization of gas phase, gas phase chemistry, and surface chemistry during high pressure vapor phase deposition processes under laminar and turbulent flow conditions."

Growth techniques that utilize elevated reactor pressures offer a pathway to overcome limitations in the epitaxy of high quality group III-nitride compounds such as InN or related materials, which exhibit large thermal decomposition pressures. We introduce the growth of InN by a unique high-pressure chemical vapor deposition (HPCVD) system, demonstrating that HPCVD is a valuable method for achieving stoichiometric single-phase surface compositions at optimal temperatures. The development and utilization of real-time optical diagnostics for the monitoring of gas-phase and surface chemistry during the heteroepitaxial nucleation and growth is critical for controlling the chemical vapor deposition process. Using real-time optical ultraviolet absorption spectroscopy (UVAS), we have studied the flow and decomposition kinetics of the gas-phase precursors as functions of flow, pressure and temperature. A pulsed-injection technique for the delivery of the chemical precursors is used, enabling the analysis and control of the decomposition kinetics of trimethylindium (TMI) and ammonia as well as the study of the initial stages of InN nucleation and subsequent overgrowth on sapphire substrates. The nucleation and steady state growth of InN is probed with sub-monolayer resolution by principal angle reflectance (PAR) spectroscopy. These real-time optical monitoring techniques demonstrate their utility in the optimization and engineering of the growth process, as well as providing crucial insights into gas phase decomposition dynamics and surface chemistry processes under HPCVD conditions. The resulting InN material exhibits an optical absorption edge that varies from 0.83 to 1.34eV, strongly dependent upon the precursor flow ratios employed during growth. Structural analysis performed by XRD reveals high quality InN.

